The WED principle and the evolution of microstructures

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BioSMA
Mathematics for Shape Memory Technologies in Biomechanics

www.imati.cnr.it/biosma

WED = Weighted Energy-Dissipation

$\longrightarrow$ variational principle for dissipative evolution systems

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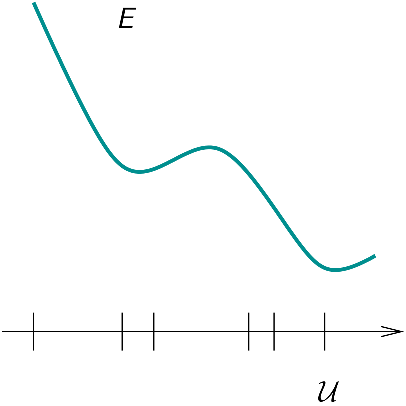
Outline

1. recall some variational tools for dissipative evolution
2. describe the WED formalism and the results
3. outline the relations with microstructure evolution

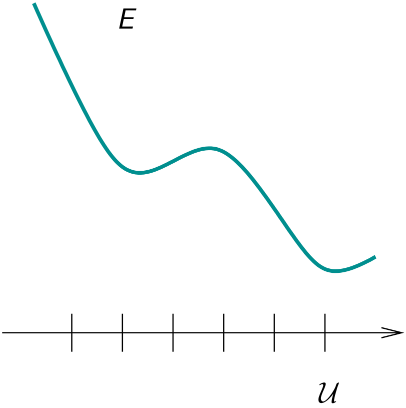
Dissipative evolution

$$\boxed{\mathrm{D}\psi(u_t) + \mathrm{D}_u E(t,u) = 0}$$



- $t \mapsto u(t) \in \mathcal{U}$ state
- $(t,u) \mapsto E(t,u)$ energy
- $\psi : \mathcal{U} \to [0,\infty]$ dissipation

Gradient flows



$E : [0, T] \times \mathcal{U} \to \mathbb{R}$ Energy

$\psi(\cdot) = \frac{1}{2}|\cdot|^2$ Dissipation

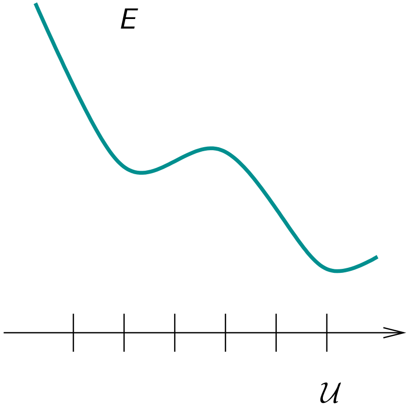
Gradient flow:

$$\begin{cases} u_t + \mathrm{D}_u E(t, u) = 0 \\ u(0) = u_0 \end{cases}$$

Gradient flows in applications

- heat, linear parabolic
- parabolic variational inequalities, ODEs with constraints
- degenerate parabolic, quasilinear, p-Laplacian
- mean curvature for graphs
- viscoelasticity
- Stefan, porous media
- reaction-diffusion, Allen-Cahn,
- phase field, Penrose-Fife systems
- ...

Rate-independent flows



$E : [0, T] \times \mathcal{U} \to \mathbb{R}$ Energy

$\psi(\cdot) = |\cdot|$ Dissipation

Rate-independent flow:

$$\begin{cases} \partial\psi(u_t) + \mathrm{D}_u E(t, u) \ni 0 \\ u(0) = u_0 \end{cases}$$

Rate-independent flows in applications

- Elastoplasticity, friction
- Damage, fractures
- ferromagnetism
- Hele-Shaw
- ...

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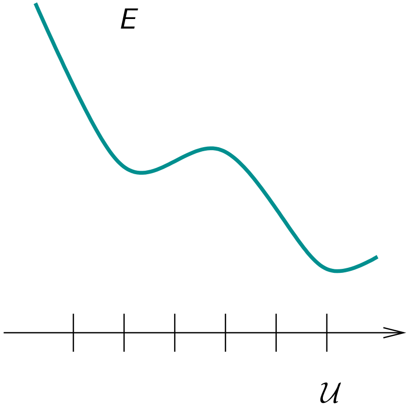
$$\partial\psi(u_t) + \mathrm{D}_u E(t,u) \ni 0, \qquad \alpha : [0,T] \to [0,T] \ \text{incr.}$$

$$\Rightarrow \quad v = u \circ \alpha \quad \text{solves} \quad \partial\psi(v_t) + \mathrm{D}_v E(\alpha(t), v) \ni 0$$

Viscous p-flows $\quad 1 < p < \infty$



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$\psi(\cdot) = \frac{1}{p} |\cdot|^p$ Dissipation

Viscous p-flow:

$$\begin{cases} |u_t|^{p-2} u_t + \mathrm{D}_u E(t, u) \ni 0 \\ u(0) = u_0 \end{cases}$$

The Aim

State dissipative evolution as a minimization over entire trajectories

$$\mathrm{D}\psi(u_t) + \mathrm{D}_u E(t,u) = 0 \quad \Longleftrightarrow \quad F(u) = \min F$$

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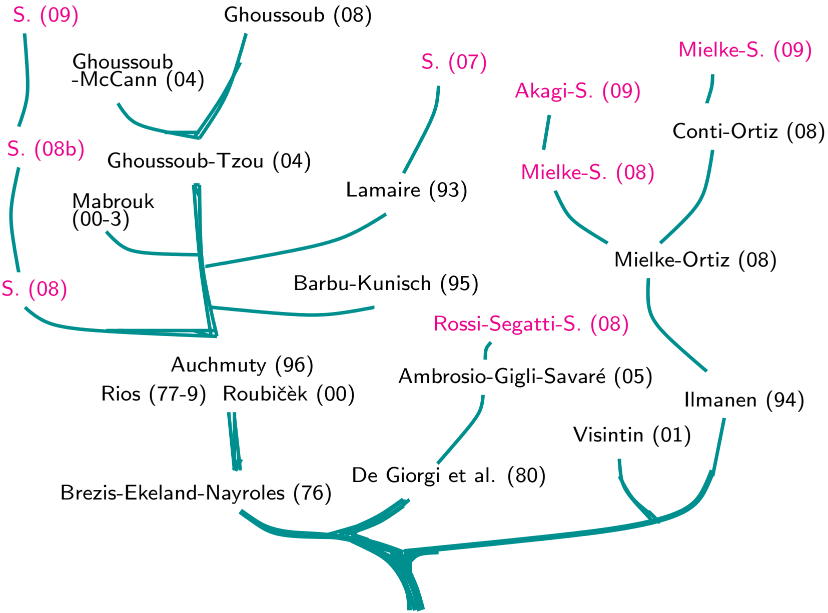
…and use the Calculus of Variations:

- Direct Method
- Γ-convergence
- relaxation
- …

Not a new idea



Three principles

for gradient flows $u_t + \mathrm{D}E(u) = 0$

Brezis-Ekeland-Nayroles' principle (76)

$$\text{minimize:} \quad u \ \mapsto \ \int_0^T \Big(E(u) + E^*(-\dot{u}) \Big) + \frac{1}{2}|u(T)|^2 - \frac{1}{2}|u_0|^2$$

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- Direct Method Nayroles (76), Rios (77-79), Auchmuty (88-93), Roubíček (00), Ghoussoub-Tzou (04)... Ghoussoub (08)
- Long-time Lemaire (96)
- Second order equations Mabrouk (00-03)
- Mild non-convexity Ghoussoub-McCann (04)

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- Doubly nonlinear, approximations, time-discrete S. (08), S. (07)
- Rate-independent, plasticity S. (08b), S. (09)

Three principles

for gradient flows $u_t + \mathrm{D}E(u) = 0$

De Giorgi's principle (80)

$$\text{minimize:} \quad u \ \mapsto \ E(u(T)) - E(u_0) + \frac{1}{2}\int_0^T |\dot{u}|^2 + \frac{1}{2}\int_0^T |\mathrm{D}E(u)|^2$$

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- Metric interpretation De Giorgi-Marino-Tosques (80), Marino-Saccon-Tosques (89), … Ambrosio-Gigli-Savaré (05)
- Doubly nonlinear version for $\psi(\dot{u}) = p(|\dot{u}|)$ Mielke, Rossi, Savaré (08)

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Three principles

for gradient flows $u_t + \mathrm{D}E(u) = 0$

Consider $F_t(u) = \dfrac{1}{2}\displaystyle\int_0^t |\dot u|^2 + E(u(t))$ and order $\{u(0) = u_0\}$ as

$$u \lesssim v \quad \text{iff} \quad \begin{cases} \text{either } u \equiv v \text{ or} \\ \text{letting } \ t_0 = \inf\{t \ : \ u(t) \neq v(t)\}, \\ F_t(u) < F_t(v) \ \text{ in } \ (t, t+\delta) \ \text{ for some } \ \delta > 0 \end{cases}$$

Visintin's principle (01)

Find a minimal element with respect to $\lesssim$

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Find a minimal element with respect to $\lesssim$

- Doubly nonlinear, no convexity
- Minimal elements generally fail to exist

The WED functional

$$W_\varepsilon(u) \; = \; \int_0^T \mathrm{e}^{-t/\varepsilon} \left(\psi(u_t) + \frac{1}{\varepsilon} E(t,u) \right) \mathrm{d}t$$

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Minimize W_ε in $\{u(0) = u_0\}$

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Minimize W_ε in $\{u(0) = u_0\}$

Euler-Lagrange equations + IC

$$-\varepsilon\partial_t \mathrm{D}\psi(u_t) + \mathrm{D}\psi(u_t) + \mathrm{D}_u E(t,u) = 0$$
$$u(0) = u_0$$
$$\mathrm{D}\psi(u_t(T)) = 0$$

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$$\begin{aligned} -\varepsilon \partial_t \mathrm{D}\psi(u_t) + \mathrm{D}\psi(u_t) + \mathrm{D}_u E(t,u) &= 0 \\ u(0) &= u_0 \\ \mathrm{D}\psi(u_t(T)) &= 0 \end{aligned}$$

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Elliptic regularization $\longrightarrow$ causal limit $\varepsilon \to 0$

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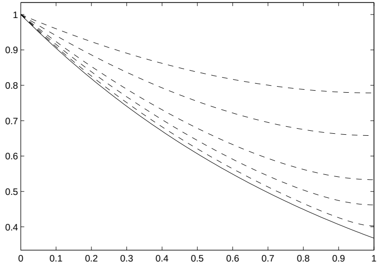
- Mielke-S. (09) — causal limit for gradient flows
- Akagi-S. — causal limit for viscous p-flows

Causal limit for gradient flows

$$\mathcal{U} = \mathbb{R}, \quad E(t,u) = \frac{1}{2}u^2, \quad u_0 = 1, \quad T = 1, \quad (u(t) = \mathrm{e}^{-t})$$

$$\boxed{W_\varepsilon(u) = \int_0^1 e^{-t/\varepsilon}\left(\frac{1}{2}\dot{u}^2 + \frac{1}{2\varepsilon}u^2\right)\mathrm{d}t}$$



The causal limit for gradient flows

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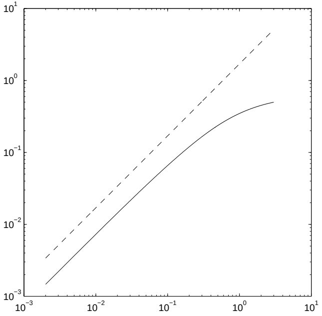

Figure: $\varepsilon \mapsto \|u - u_\varepsilon\|_{C[0,T]}$

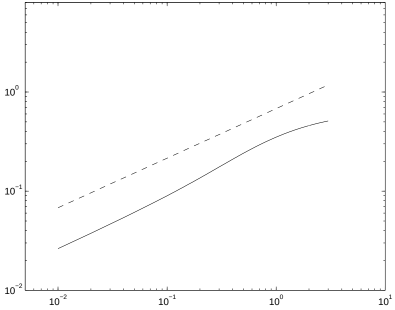

Figure: $\varepsilon \mapsto \|u - u_\varepsilon\|_{H^1(0,T)}$

Causal limit for gradient flows

space: $\mathcal{U} =$ Hilbert

dissip.: $\psi(\dot{u}) = \frac{1}{2}\|\dot{u}\|^2_{\mathcal{U}}$

energy: $E(t,u) = \phi(u)$ — ϕ is λ-convex, proper, l.s.c.

datum: $\phi(u_0) < \infty$

Mielke-S.

$$u_\varepsilon(t) \to u(t) \qquad \text{uniformly}$$

where u solves the gradient flow

$$u_t + \partial\phi(u) \ni 0$$

Causal limit for gradient flows

More precisely:

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- sharp rate estimate

$$\max_t \|u(t) - u_\varepsilon(t)\|_{\mathcal{U}} \;\leq\; c\,\varepsilon^{1/2}$$

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$$\max_t \|u(t) - u_\varepsilon(t)\|_{\mathcal{U}} \ \leq \ c\,\varepsilon^{1/2}$$

- convergence in H^s, $s < 1$

$$\|u - u_\varepsilon\|_{H^s(0,T;\mathcal{U})} \ \leq \ c\,\varepsilon^{(1-s)/2}$$

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- more general data

$$u_0 \notin D(\phi) \ \subset \ \overline{D(\phi)}, \qquad \text{r.h.s.} \ \ f \in L^2(0,T;\mathcal{U})$$

Causal limit for rate-independent problems

space: $\mathcal{U} =$ Banach

dissip.: $\psi(\dot{u}) \geq c_\psi \|\dot{u}\|_{\mathcal{U}}$

energy: $E(t, u)$ weakly l.s.c., compact sublevels, smooth in t

datum: $\phi(u_0) < E(0, u) + \psi(u - u_0) \quad \forall u \in \mathcal{U}$

Mielke-Ortiz 08

$$u_\varepsilon(t) \to u(t) \qquad \text{pointwise}$$

where u solves in an energetic solution of the rate-independent problem $\partial\psi(u_t) + \mathrm{D}E(t, u) \ni 0$ and $u(0) = u_0$

Causal limit for viscous p-flows $(1 < p < \infty)$

space: $\mathcal{U} = L^p(\Omega)$

dissip.: $\psi(u_t) = \frac{1}{p}\int_\Omega |u_t|^p$

energy: $E(t,u) = \int_\Omega \left(\frac{1}{q}|\nabla u|^q + \phi(u)\right)$ $(p < q^*)$

datum: u_0 smooth

Akagi-S.

$$u_\varepsilon(t) \to u(t) \qquad \text{uniformly in } L^p(\Omega)$$

where u solves the doubly nonlinear relation

$$|u_t|^{p-2}u_t - \Delta_q u + \partial\phi(u) \ni 0.$$

Microstructures

$E : L^2(-1,1) \to (-\infty, \infty]$ energy

$$E(u) = \begin{cases} \frac{1}{2}\int_{-1}^{1} u^2 & \text{if } \ |u_x| = 1 \ \text{ a.e.} \\ \infty & \text{else} \end{cases}$$

$$\boxed{\min\{E(u) \ : \ u(-1) = u(1) = 0\}}$$

Relaxation

$$\mathrm{sc}^- E(u) = \begin{cases} \dfrac{1}{2}\displaystyle\int_{-1}^{1} u^2 & \text{if } \; |u_x| \leq 1 \; \text{ a.e.} \\ \infty & \text{else} \end{cases}$$

$$\boxed{\min\{\mathrm{sc}^- E(u) \; : \; u(-1) = u(1) = 0\}}$$

Microstructure evolution

gradient flow

$$\boxed{u_t + \mathrm{D}_u E(u) = 0}$$

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Variational program

1. Minimize W_ε

Microstructure evolution

gradient flow

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Variational program

1. Minimize W_ε $\longrightarrow$ Relax W_ε $\longrightarrow$ Minimize $\mathrm{sc}^- W_\varepsilon$

Microstructure evolution

gradient flow

$$\boxed{u_t + \mathrm{D}_u E(u) = 0}$$

Variational program

1. Minimize W_ε $\longrightarrow$ Relax W_ε $\longrightarrow$ Minimize $\mathrm{sc}^- W_\varepsilon$
2. Take $\varepsilon \to 0$

The Conti-Ortiz example

$$\mathcal{U} = L^2(-1,1)$$

$$\psi(u_t) = \frac{1}{2}\int_{-1}^{1} u_t^2(x)\,\mathrm{d}x$$

$$E(t,u) = \begin{cases} -\displaystyle\int_{-1}^{1} f(t,x)\,u(x)\,\mathrm{d}x & \text{if } |u_x| = 1 \text{ a.e.} \\ \infty & \text{else} \end{cases}$$

The Conti-Ortiz example

The corresponding WED functional

$$W_\varepsilon(u) = \begin{cases} \displaystyle\int_0^T\int_{-1}^1 \mathrm{e}^{-t/\varepsilon}\left(\frac{1}{2}u_t^2 - \frac{1}{\varepsilon}fu\right)\mathrm{d}x\,\mathrm{d}t & \text{if } \ |u_x| = 1 \ \text{ a.e.} \\ \infty & \text{else} \end{cases}$$

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and its relaxation w.r.t. the weak topology of H^1 in $\{u(0,\cdot) = 0\}$ is

$$\mathrm{sc}^- W_\varepsilon(u) = \begin{cases} \displaystyle\int_0^T \int_{-1}^1 \mathrm{e}^{-t/\varepsilon} \left(\frac{1}{2} u_t^2 - \frac{1}{\varepsilon} f u \right) \mathrm{d}x \, \mathrm{d}t & \text{if } |u_x| \leq 1 \text{ a.e.} \\ \infty & \text{else} \end{cases}$$

The Conti-Ortiz example

The relaxation corresponds to

$$E_{\mathrm{eff}}(t,u) = \int_{-1}^{1} \Big(I_{[-1,1]}(u_x(x)) - f(t,x)\, u(x) \Big) \mathrm{d}x$$

The Conti-Ortiz example

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The effective evolution:

$$\boxed{u_t + \partial_u E_{\text{eff}}(t,u) \ni 0}$$

Conjecture (Conti-Ortiz (08))

$$u_\varepsilon \longrightarrow u\,?$$

The Conti-Ortiz example

Minimizers of $\mathrm{sc}^- W_\varepsilon$ converge

$$\mathrm{sc}^- W_\varepsilon(u_\varepsilon) \equiv \min \quad \Longrightarrow \quad u_\varepsilon \to u$$

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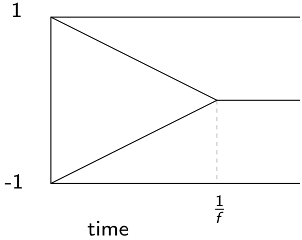
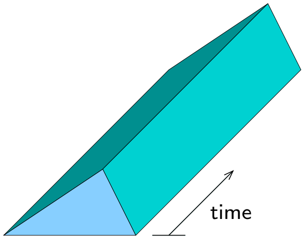
Quasi-minimizers of W_ε converge

$$W_\varepsilon(v_\varepsilon) \leq \inf W_\varepsilon + \varepsilon^3 \mathrm{e}^{-T/\varepsilon} \quad \Longrightarrow \quad v_\varepsilon \to u$$

The Conti-Ortiz example

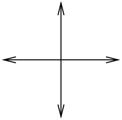
An illustration of microstructure evolution for a fixed $f > 0$





A second example by Conti-Ortiz

$$Q = [0,1]^2, \quad K = \{(0,\pm1),(\pm1,0)\} =$$



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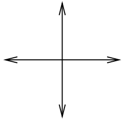

$$W_\varepsilon(u) = \begin{cases} \displaystyle\int_0^T \int_Q \mathrm{e}^{-t/\varepsilon} \left(\frac{1}{2} u_t^2 - \frac{1}{\varepsilon} f u \right) \mathrm{d}x \, \mathrm{d}t & \text{if } \nabla u \in K \text{ a.e.} \\ \infty & \text{else} \end{cases}$$

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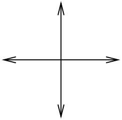
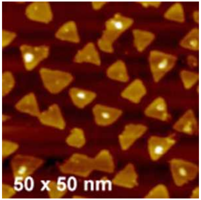
$$Q = [0,1]^2, \quad K = \{(0,\pm 1), (\pm 1, 0)\} =$$



$$W_\varepsilon(u) = \begin{cases} \displaystyle\int_0^T \int_Q \mathrm{e}^{-t/\varepsilon} \left(\frac{1}{2} u_t^2 - \frac{1}{\varepsilon} f u \right) \mathrm{d}x \, \mathrm{d}t & \text{if } \nabla u \in K \text{ a.e.} \\ \infty & \text{else} \end{cases}$$

Roughening and coarsening in thin films
Ortiz, Repetto, Si (99)

(vanishing capillarity case)



A second example by Conti-Ortiz

The relaxation w.r.t. the weak topology of H^1 in $\{u(0,\cdot)=0\}$ is

$$\mathrm{sc}^- W_\varepsilon(u) = \begin{cases} \displaystyle\int_0^T\!\!\int_Q \mathrm{e}^{-t/\varepsilon}\left(\frac{1}{2}u_t^2 - \frac{1}{\varepsilon}fu\right)\mathrm{d}x\,\mathrm{d}t & \text{if } \nabla u \in \mathrm{co}\,K \text{ a.e.} \\ \infty & \text{else} \end{cases}$$

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which corresponds to

$$E_{\mathrm{eff}}(t,u) = \int_Q \Big(I_{\mathrm{co}K}(\nabla u(x)) - f(t,x)\, u(x)\Big)\mathrm{d}x$$

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Minimizers of $\mathrm{sc}^- W_\varepsilon$ converge

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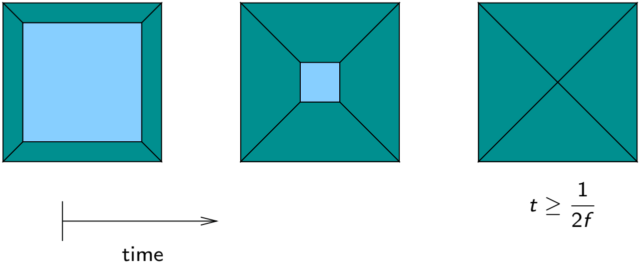
Quasi-minimizers of W_ε converge

$$W_\varepsilon(v_\varepsilon) \le \inf W_\varepsilon + \varepsilon^3 \mathrm{e}^{-T/\varepsilon} \quad \Longrightarrow \quad v_\varepsilon \to u$$

A second example by Conti-Ortiz

An illustration of microstructure evolution for a fixed $f > 0$



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- The corresponding minimizers converge to the right limit by assuming a convex energy (for $p \neq 1$) and compactness (for $p \neq 2$)
- The WED principle serves as a tool in connection with some example of microstructure evolution